



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:13 am GMT

PDB ID : 2WYN  
Title : STRUCTURE OF FAMILY 37 TREHALASE FROM ESCHERICHIA COLI  
IN COMPLEX WITH A CASUARINE-6-O-A-D-GLUCOSIDE ANALOGUE  
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giani, C.; Parenti, P.; Fusi, P.; Forcella, M.; Cipolla, L.  
Deposited on : 2009-11-17  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

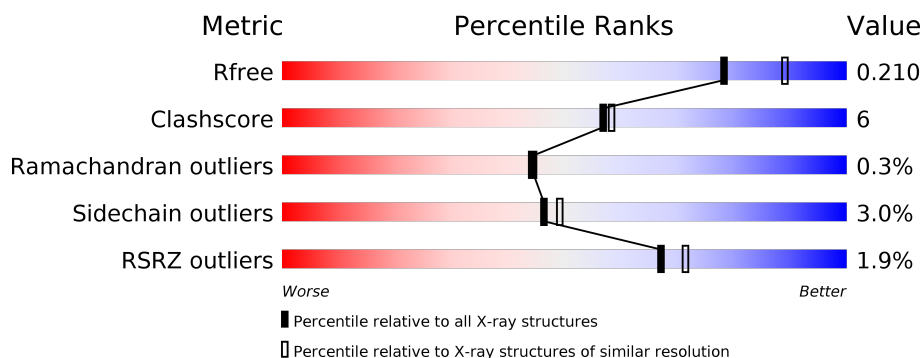
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>2%</div> <div>83% 12% 5%</div> </div>
1	B	535	<div> <div>2%</div> <div>82% 10% 6%</div> </div>
1	C	535	<div> <div>2%</div> <div>84% 8% 6%</div> </div>
1	D	535	<div> <div>2%</div> <div>82% 11% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	1555	-	-	-	X
4	SO4	B	1549	-	-	X	-
4	SO4	C	1553	-	-	-	X
4	SO4	C	1555	-	-	-	X

## 2 Entry composition [i](#)

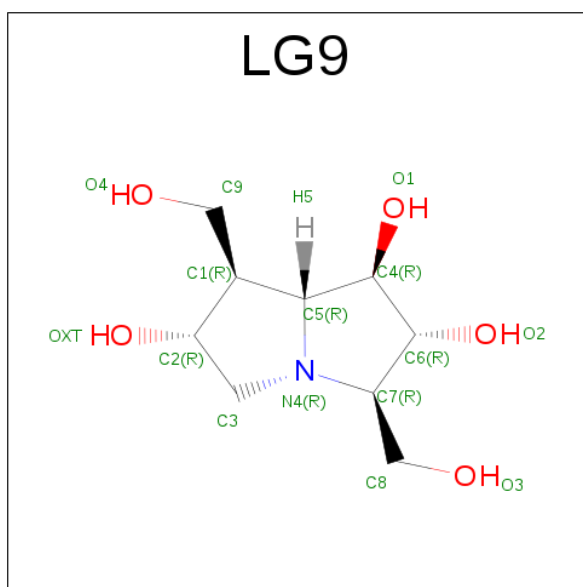
There are 6 unique types of molecules in this entry. The entry contains 18124 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PERIPLASMIC TREHALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	18	0
			4134	2628	707	781	18			
1	B	503	Total	C	N	O	S	0	10	0
			4079	2595	696	770	18			
1	C	501	Total	C	N	O	S	0	10	0
			4049	2576	694	761	18			
1	D	503	Total	C	N	O	S	0	9	0
			4034	2573	682	761	18			

- Molecule 2 is (1R,2R,3R,6R,7R,7AR)-3,7-BIS(HYDROXYMETHYL)HEXAHYDRO-1H-PYRROLIZINE-1,2,6-TRIOL (three-letter code: LG9) (formula: C<sub>9</sub>H<sub>17</sub>NO<sub>5</sub>).



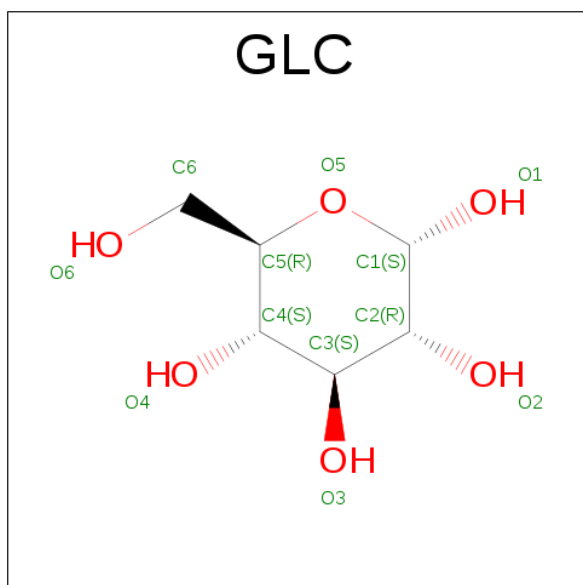
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	9	1	4		
2	B	1	Total	C	N	O	0	0
			14	9	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	9	1	4		
2	D	1	Total	C	N	O	0	0
			14	9	1	4		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE) (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0

- Molecule 6 is water.

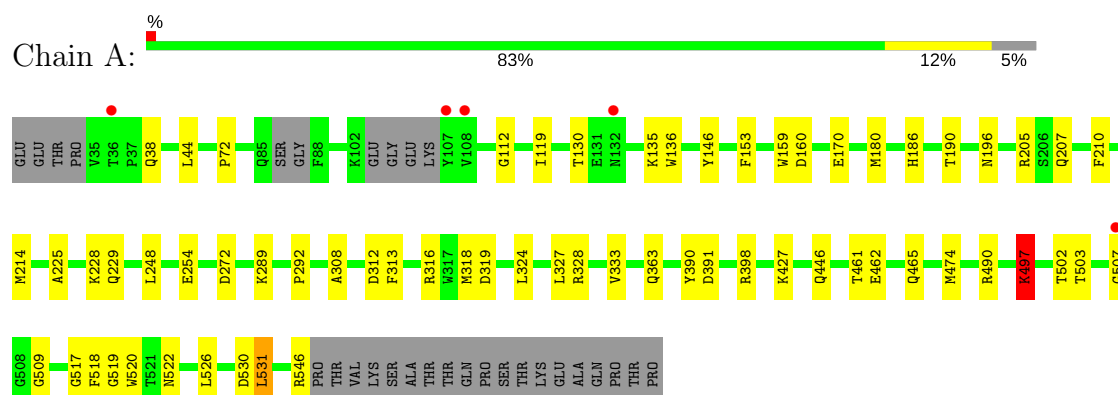
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	381	Total 398	O 398	0	17
6	B	429	Total 442	O 442	0	13
6	C	365	Total 379	O 379	0	14
6	D	333	Total 344	O 344	0	11



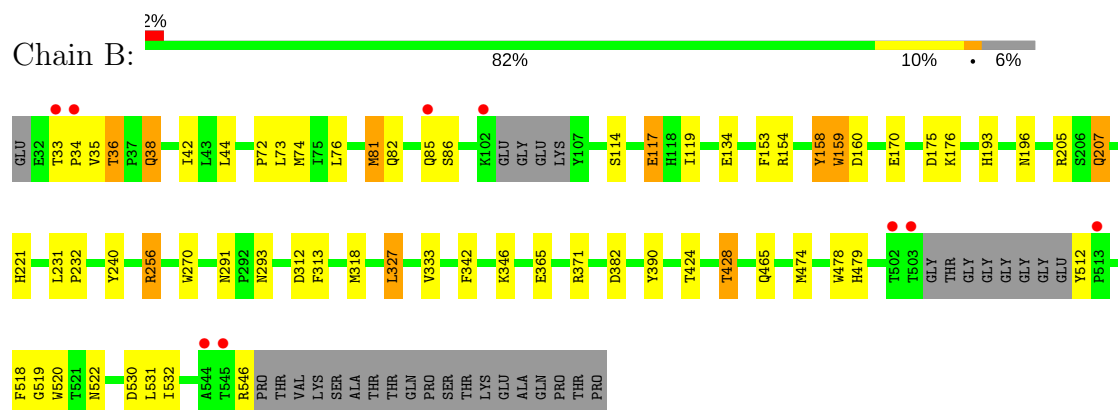
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

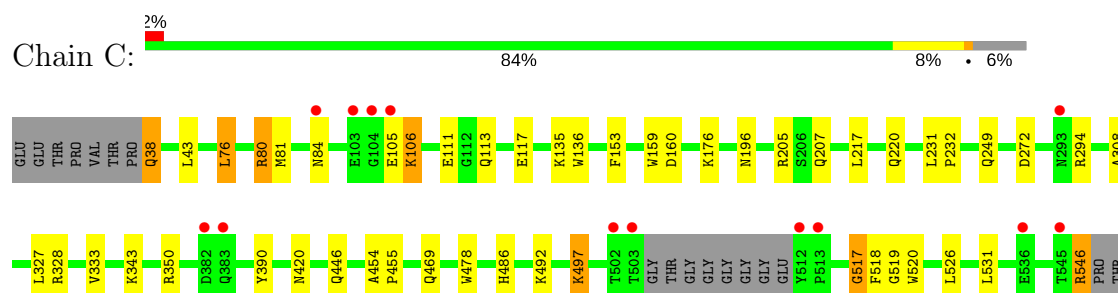
#### • Molecule 1: PERIPLASMIC TREHALASE



#### • Molecule 1: PERIPLASMIC TREHALASE

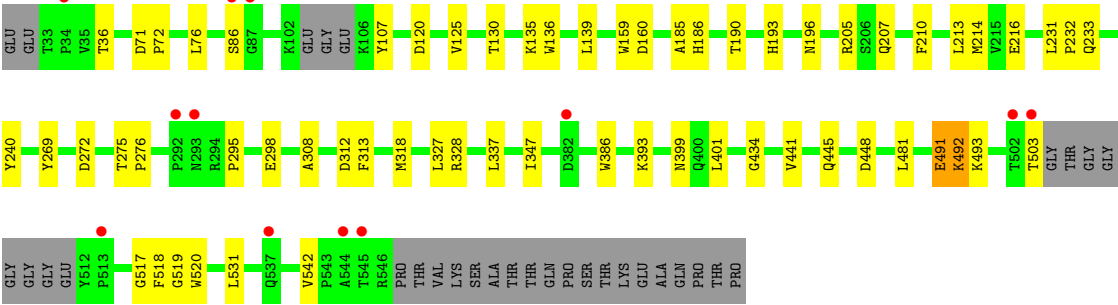
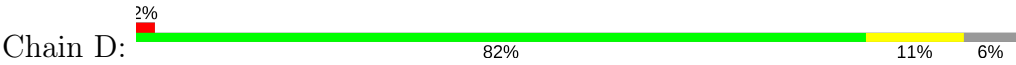


#### • Molecule 1: PERIPLASMIC TREHALASE



VAL
LYS
ALA
THR
GLN
PRO
SER
THR
LYS
GLU
ALA
GLN
PRO
THR
PRO

● Molecule 1: PERIPLASMIC TREHALASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.35Å 117.02Å 203.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.53 – 2.10 20.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (101.53-2.10) 99.7 (20.03-2.10)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.159 , 0.209 0.160 , 0.210	Depositor DCC
$R_{free}$ test set	6578 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18124	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC, LG9, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.68	0/4295	0.70	3/5854 (0.1%)
1	B	0.71	1/4222 (0.0%)	0.70	0/5756
1	C	0.66	1/4191 (0.0%)	0.70	3/5712 (0.1%)
1	D	0.62	0/4174	0.68	0/5698
All	All	0.67	2/16882 (0.0%)	0.69	6/23020 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	117	GLU	CD-OE2	6.54	1.32	1.25
1	C	117	GLU	CG-CD	5.24	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	294	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	112	GLY	N-CA-C	5.45	126.72	113.10
1	A	497	LYS	CD-CE-NZ	5.22	123.70	111.70
1	C	328[A]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	328[B]	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4134	0	3947	50	0
1	B	4079	0	3916	61	0
1	C	4049	0	3871	33	0
1	D	4034	0	3832	53	0
2	A	14	0	15	2	0
2	B	14	0	15	2	0
2	C	14	0	15	1	0
2	D	14	0	15	0	0
3	A	12	0	11	1	0
3	B	12	0	11	0	0
3	C	12	0	11	0	0
3	D	12	0	11	0	0
4	A	45	0	0	1	0
4	B	40	0	0	5	0
4	C	35	0	0	1	0
4	D	40	0	0	1	0
5	A	1	0	0	0	0
6	A	398	0	0	4	0
6	B	442	0	0	8	0
6	C	379	0	0	3	0
6	D	344	0	0	4	0
All	All	18124	0	15670	184	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38[A]:GLN:NE2	6:A:2005:HOH:O	1.68	1.22
1:A:229[B]:GLN:OE1	6:A:2174:HOH:O	1.54	1.22
1:C:76:LEU:HD13	1:C:80[B]:ARG:HH21	1.22	0.99
1:C:196:ASN:HD22	1:C:205:ARG:HE	1.19	0.91
1:C:136:TRP:HH2	6:C:2030:HOH:O	1.53	0.90
1:D:136:TRP:HH2	6:D:2026:HOH:O	1.56	0.89
1:A:130:THR:HG22	1:A:130:THR:O	1.74	0.85
1:C:76:LEU:CD1	1:C:80[B]:ARG:NH2	2.40	0.84
1:C:76:LEU:HD13	1:C:80[B]:ARG:NH2	1.93	0.83
1:B:38:GLN:HG2	1:B:42:ILE:HG21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ASN:HD22	1:D:205:ARG:HE	1.30	0.79
1:C:76:LEU:CD1	1:C:80[B]:ARG:HH21	1.94	0.78
1:A:196:ASN:HD22	1:A:205:ARG:HE	1.31	0.78
1:B:196:ASN:HD22	1:B:205:ARG:HE	1.29	0.78
1:A:446:GLN:NE2	1:A:497:LYS:HE2	2.00	0.76
1:A:363:GLN:HE22	1:C:84:ASN:HD21	1.34	0.75
1:B:291:ASN:OD1	1:B:293:ASN:HB2	1.89	0.73
1:B:478:TRP:CE2	1:B:546:ARG:HD3	2.26	0.71
1:B:74:MET:CE	1:D:232:PRO:CB	2.69	0.70
1:D:71:ASP:HA	1:D:136:TRP:CZ2	2.26	0.70
1:C:446:GLN:NE2	1:C:497:LYS:HE2	2.07	0.70
1:C:136:TRP:CH2	6:C:2030:HOH:O	2.34	0.70
1:B:38:GLN:HG2	1:B:42:ILE:CG2	2.21	0.69
1:A:398[B]:ARG:HD2	6:A:2288:HOH:O	1.92	0.68
1:B:424:THR:O	1:B:428:THR:HG23	1.94	0.67
1:C:196:ASN:ND2	1:C:205:ARG:HE	1.90	0.67
1:B:158:TYR:HB3	1:B:207:GLN:HE21	1.61	0.66
1:C:76:LEU:HD11	1:C:80[B]:ARG:NH2	2.10	0.65
1:A:446:GLN:HE21	1:A:497:LYS:HZ3	1.46	0.64
1:B:44:LEU:HD23	1:B:72:PRO:HB3	1.79	0.64
1:B:73:LEU:HD23	1:B:74:MET:HE2	1.79	0.63
1:A:328:ARG:NH1	1:A:391:ASP:OD2	2.27	0.62
1:B:256[A]:ARG:NH1	4:B:1550:SO4:O2	2.33	0.62
1:B:74:MET:HE1	1:D:232:PRO:CB	2.29	0.62
1:D:135:LYS:O	1:D:136:TRP:HB2	2.01	0.61
1:B:512:TYR:N	6:B:2406:HOH:O	2.33	0.61
1:A:130:THR:CG2	1:A:130:THR:O	2.48	0.60
1:C:196:ASN:HD22	1:C:205:ARG:NE	1.94	0.59
1:D:72:PRO:HD3	1:D:136:TRP:CE2	2.38	0.59
1:A:135[A]:LYS:HE3	1:A:136[A]:TRP:CZ2	2.38	0.57
1:B:221:HIS:HD2	6:B:2171:HOH:O	1.85	0.57
1:A:446:GLN:HE21	1:A:497:LYS:HE2	1.68	0.57
1:B:36:THR:HG21	1:D:36:THR:OG1	2.03	0.57
1:C:478:TRP:CE2	1:C:546:ARG:HD3	2.39	0.57
1:B:74:MET:HE3	1:D:232:PRO:HB2	1.85	0.57
1:B:74:MET:HA	1:B:74:MET:HE2	1.87	0.56
1:D:272:ASP:OD2	4:D:1549:SO4:O3	2.24	0.56
1:A:461:THR:O	1:A:465[B]:GLN:HG3	2.07	0.55
1:D:72:PRO:HD2	1:D:136:TRP:NE1	2.20	0.55
1:B:474:MET:HE3	1:B:532:ILE:HG22	1.87	0.55
1:C:111:GLU:O	1:C:492:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:MET:HE1	1:B:82:GLN:HG2	1.89	0.55
1:D:186:HIS:ND1	6:D:2067[B]:HOH:O	2.33	0.55
1:A:146:TYR:CB	1:A:180[A]:MET:SD	2.95	0.54
1:A:272:ASP:OD2	4:A:1550:SO4:O4	2.25	0.54
1:D:216[B]:GLU:OE2	1:D:347:ILE:HG23	2.08	0.54
1:B:196:ASN:ND2	1:B:205:ARG:HE	2.03	0.53
1:A:502:THR:O	1:A:503:THR:OG1	2.16	0.53
1:B:33:THR:CG2	1:B:34:PRO:HD2	2.39	0.53
1:C:446:GLN:NE2	1:C:497:LYS:CE	2.71	0.53
1:A:146:TYR:HA	1:A:180[A]:MET:SD	2.50	0.52
1:A:462:GLU:OE2	1:A:465[B]:GLN:OE1	2.27	0.52
1:B:478:TRP:NE1	1:B:546:ARG:HD3	2.23	0.52
1:A:170:GLU:OE2	1:A:530:ASP:OD2	2.28	0.52
1:A:225:ALA:HA	1:A:228:LYS:HE3	1.92	0.52
1:B:176:LYS:HG3	6:B:2175:HOH:O	2.08	0.52
1:B:175:ASP:HB2	4:B:1549:SO4:O3	2.10	0.52
1:D:72:PRO:CD	1:D:136:TRP:CD1	2.93	0.52
1:B:74:MET:HE1	1:D:232:PRO:HB3	1.91	0.52
1:C:113:GLN:NE2	6:C:2068:HOH:O	2.28	0.52
1:A:465[B]:GLN:HE22	1:A:531:LEU:HD21	1.74	0.52
1:B:74:MET:HE1	1:D:232:PRO:CG	2.40	0.51
1:D:72:PRO:CD	1:D:136:TRP:NE1	2.73	0.51
1:B:231:LEU:HB3	1:B:232:PRO:HD3	1.92	0.51
1:A:146:TYR:HB2	1:A:180[A]:MET:SD	2.50	0.51
1:B:159:TRP:H	1:B:207:GLN:NE2	2.08	0.51
1:D:295:PRO:HD2	1:D:298[A]:GLU:OE2	2.11	0.50
1:A:446:GLN:HE21	1:A:497:LYS:NZ	2.08	0.50
1:A:186:HIS:O	1:A:190:THR:HG23	2.11	0.50
1:B:175:ASP:HB2	4:B:1549:SO4:O1	2.11	0.50
1:B:153:PHE:CZ	2:B:1547:LG9:H32C	2.47	0.49
1:B:176:LYS:NZ	6:B:2174:HOH:O	2.44	0.49
1:B:346:LYS:NZ	1:B:365:GLU:OE2	2.33	0.49
1:A:292:PRO:HB3	1:C:249[A]:GLN:NE2	2.27	0.49
1:A:465[B]:GLN:NE2	1:A:531:LEU:HD11	2.27	0.49
1:B:81:MET:CE	1:B:85:GLN:HE22	2.25	0.49
1:D:130:THR:HG21	1:D:139:LEU:HD21	1.94	0.49
1:B:74:MET:CE	1:D:232:PRO:HB3	2.42	0.49
1:B:74:MET:HE3	1:D:232:PRO:CB	2.41	0.49
1:D:481:LEU:HB3	1:D:542:VAL:HG21	1.95	0.49
1:A:207:GLN:HA	1:A:308:ALA:O	2.13	0.48
1:A:196:ASN:ND2	1:A:205:ARG:HE	2.07	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:CE	1:B:74:MET:HA	2.44	0.48
1:A:446:GLN:HE21	1:A:497:LYS:CE	2.26	0.48
1:C:207:GLN:HA	1:C:308:ALA:O	2.13	0.48
1:A:465[B]:GLN:HE22	1:A:531:LEU:HD11	1.79	0.48
1:D:328:ARG:NH2	1:D:393:LYS:HG3	2.27	0.48
1:D:185:ALA:HB1	1:D:233:GLN:HG2	1.96	0.48
1:B:153:PHE:CE1	2:B:1547:LG9:H32C	2.48	0.48
1:B:193:HIS:HB3	1:B:240:TYR:CD1	2.49	0.48
1:B:74:MET:CE	1:D:232:PRO:HB2	2.40	0.47
1:A:196:ASN:HD22	1:A:205:ARG:NE	2.08	0.47
1:D:434:GLY:HA2	1:D:503:THR:HG22	1.96	0.47
1:B:342:PHE:HB2	1:B:371:ARG:HG2	1.96	0.47
1:D:491:GLU:O	1:D:492:LYS:HB2	2.13	0.47
1:A:153:PHE:CE1	2:A:1547:LG9:H32C	2.49	0.47
1:A:363:GLN:HE22	1:C:84:ASN:ND2	2.08	0.47
1:B:36:THR:CG2	1:D:36:THR:OG1	2.62	0.47
1:D:441:VAL:O	1:D:448:ASP:HB3	2.14	0.47
1:D:196:ASN:ND2	1:D:205:ARG:HE	2.06	0.47
1:B:196:ASN:HD22	1:B:205:ARG:NE	2.07	0.46
1:C:478:TRP:CH2	1:C:546:ARG:HB2	2.51	0.46
1:B:81:MET:HE3	1:B:85:GLN:HE22	1.81	0.46
1:C:111:GLU:O	1:C:492:LYS:CE	2.63	0.45
1:D:72:PRO:HD3	1:D:136:TRP:CD2	2.50	0.45
1:B:114:SER:HG	1:B:117:GLU:CD	2.19	0.45
1:B:478:TRP:CH2	1:B:546:ARG:HA	2.51	0.45
1:C:105:GLU:C	1:C:106:LYS:HG3	2.37	0.45
1:A:135[A]:LYS:O	1:A:136[A]:TRP:HB2	2.16	0.45
1:A:153:PHE:CZ	2:A:1547:LG9:H32C	2.52	0.45
1:A:248:LEU:HD13	1:A:254:GLU:CG	2.46	0.45
1:D:231:LEU:N	1:D:232:PRO:CD	2.80	0.45
1:A:446:GLN:HE22	1:A:497:LYS:HE2	1.80	0.45
1:C:231:LEU:HB3	1:C:232:PRO:HD3	1.99	0.45
1:B:35:VAL:HG21	1:D:190[A]:THR:HG22	1.99	0.44
1:D:72:PRO:CD	1:D:136:TRP:CE2	3.00	0.44
1:A:319:ASP:OD1	1:A:328:ARG:NE	2.40	0.44
1:C:153:PHE:CZ	2:C:1547:LG9:H32C	2.52	0.44
1:B:333:VAL:HB	1:B:390:TYR:HB3	1.99	0.44
1:C:272:ASP:OD2	4:C:1549:SO4:O3	2.35	0.44
1:D:269:TYR:CZ	1:D:337:LEU:HB2	2.53	0.44
1:D:492:LYS:HD2	1:D:492:LYS:N	2.32	0.44
1:A:44:LEU:HD23	1:A:72:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:MET:HE1	1:A:531:LEU:HD22	2.00	0.44
1:B:158:TYR:HB3	1:B:207:GLN:HB2	2.00	0.44
1:D:136:TRP:CH2	6:D:2026:HOH:O	2.45	0.44
1:C:343:LYS:HA	1:C:343:LYS:HD2	1.86	0.43
1:C:38:GLN:HB3	1:C:43:LEU:HD13	2.00	0.43
1:D:386:TRP:CE2	1:D:401:LEU:HB2	2.53	0.43
4:B:1551:SO4:O1	6:B:2438:HOH:O	2.21	0.43
1:B:546:ARG:HD2	6:B:2191:HOH:O	2.19	0.43
1:D:207:GLN:HA	1:D:308:ALA:O	2.18	0.43
1:C:217:LEU:O	1:C:220:GLN:HB2	2.19	0.43
1:C:420:ASN:OD1	1:C:469:GLN:NE2	2.48	0.43
1:D:318[B]:MET:CE	1:D:445:GLN:HG3	2.49	0.43
1:B:170:GLU:OE2	1:B:530:ASP:OD2	2.37	0.43
1:B:465[A]:GLN:NE2	6:B:2382:HOH:O	2.44	0.42
1:A:333:VAL:HB	1:A:390:TYR:HB3	2.00	0.42
1:D:71:ASP:HA	1:D:136:TRP:CE2	2.53	0.42
1:B:256[A]:ARG:HG3	1:B:270:TRP:HB3	2.01	0.42
1:B:176:LYS:HA	1:B:176:LYS:HD3	1.85	0.42
1:D:312:ASP:HA	1:D:313:PHE:HA	1.83	0.42
1:A:196:ASN:ND2	3:A:1548:GLC:O3	2.53	0.42
1:A:517:GLY:HA3	1:A:518:PHE:HA	1.87	0.42
1:B:312:ASP:HA	1:B:313:PHE:HA	1.87	0.42
1:B:518:PHE:O	1:B:519:GLY:C	2.58	0.42
1:D:107:TYR:CD1	1:D:125:VAL:HG21	2.55	0.42
1:D:213:LEU:HD12	1:D:213:LEU:N	2.35	0.41
1:D:275:THR:HB	1:D:276:PRO:CD	2.50	0.41
1:D:193:HIS:HB3	1:D:240:TYR:CD1	2.55	0.41
1:A:318:MET:HE3	1:A:324:LEU:HA	2.01	0.41
1:D:72:PRO:CG	1:D:136:TRP:CD1	3.04	0.41
1:A:427:LYS:HG2	6:A:2153:HOH:O	2.19	0.41
1:B:154:ARG:HD3	6:B:2156:HOH:O	2.20	0.41
1:D:120:ASP:HB3	6:D:2121:HOH:O	2.20	0.41
1:D:210:PHE:O	1:D:214:MET:HG3	2.21	0.41
1:B:73:LEU:HD23	1:B:74:MET:CE	2.47	0.41
1:A:119:ILE:HG23	1:A:522:ASN:HB3	2.02	0.41
1:A:474:MET:HE1	1:A:531:LEU:HD13	2.03	0.41
1:D:481:LEU:HB3	1:D:542:VAL:CG2	2.50	0.41
1:A:312:ASP:HA	1:A:313:PHE:HA	1.81	0.41
1:B:175:ASP:HB2	4:B:1549:SO4:S	2.61	0.41
1:C:135:LYS:O	1:C:136:TRP:HB2	2.21	0.41
1:C:333:VAL:HB	1:C:390:TYR:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:LEU:HB3	1:D:232:PRO:HD3	2.02	0.41
1:B:119:ILE:HG23	1:B:522:ASN:HB3	2.03	0.40
1:D:517:GLY:HA3	1:D:518:PHE:HA	1.83	0.40
1:A:210:PHE:O	1:A:214:MET:HG3	2.21	0.40
1:C:454:ALA:N	1:C:455:PRO:HD2	2.36	0.40
1:B:318:MET:HA	1:B:327:LEU:HA	2.03	0.40
1:C:517:GLY:HA3	1:C:518:PHE:HA	1.78	0.40
1:D:491:GLU:HB3	1:D:493:LYS:HG2	2.04	0.40
1:A:507:GLY:C	1:A:509:GLY:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/535 (97%)	505 (98%)	12 (2%)	1 (0%)	51	52
1	B	507/535 (95%)	496 (98%)	10 (2%)	1 (0%)	51	52
1	C	507/535 (95%)	493 (97%)	12 (2%)	2 (0%)	38	35
1	D	506/535 (95%)	492 (97%)	12 (2%)	2 (0%)	38	35
All	All	2038/2140 (95%)	1986 (97%)	46 (2%)	6 (0%)	44	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	86	SER
1	A	519	GLY
1	B	158	TYR
1	C	519	GLY
1	D	519	GLY
1	C	517	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	437/456 (96%)	426 (98%)	11 (2%)	53	57
1	B	437/456 (96%)	421 (96%)	16 (4%)	39	39
1	C	428/456 (94%)	409 (96%)	19 (4%)	33	31
1	D	424/456 (93%)	415 (98%)	9 (2%)	59	64
All	All	1726/1824 (95%)	1671 (97%)	55 (3%)	46	46

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	TRP
1	A	160	ASP
1	A	289	LYS
1	A	327	LEU
1	A	490[A]	ARG
1	A	490[B]	ARG
1	A	497	LYS
1	A	520	TRP
1	A	526	LEU
1	A	531	LEU
1	A	546	ARG
1	B	36	THR
1	B	38	GLN
1	B	76	LEU
1	B	81	MET
1	B	86	SER
1	B	134	GLU
1	B	159	TRP
1	B	160	ASP
1	B	207	GLN
1	B	256[A]	ARG
1	B	256[B]	ARG
1	B	327	LEU
1	B	428	THR

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Mol	Chain	Res	Type
1	B	479	HIS
1	B	520	TRP
1	B	531	LEU
1	C	38	GLN
1	C	76	LEU
1	C	80[A]	ARG
1	C	80[B]	ARG
1	C	81[A]	MET
1	C	81[B]	MET
1	C	106	LYS
1	C	159	TRP
1	C	160	ASP
1	C	176	LYS
1	C	327	LEU
1	C	350	ARG
1	C	486[A]	HIS
1	C	486[B]	HIS
1	C	497	LYS
1	C	520	TRP
1	C	526	LEU
1	C	531	LEU
1	C	546	ARG
1	D	76	LEU
1	D	159	TRP
1	D	160	ASP
1	D	327	LEU
1	D	399	ASN
1	D	491	GLU
1	D	492	LYS
1	D	520	TRP
1	D	531	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	235	GLN
1	A	261	GLN
1	A	400	GLN
1	A	446	GLN
1	B	38	GLN
1	B	82	GLN

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Mol	Chain	Res	Type
1	B	113	GLN
1	B	196	ASN
1	B	207	GLN
1	B	221	HIS
1	B	249	GLN
1	B	293	ASN
1	B	400	GLN
1	B	429	HIS
1	B	479	HIS
1	C	84	ASN
1	C	196	ASN
1	C	446	GLN
1	C	465	GLN
1	D	82	GLN
1	D	113	GLN
1	D	196	ASN
1	D	293	ASN
1	D	384	GLN
1	D	469	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 1 is monoatomic - leaving 40 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	LG9	A	1547	3	15,15,16	1.05	0	17,22,24	2.41	7 (41%)
3	GLC	A	1548	2	12,12,12	0.57	0	17,17,17	0.92	0
4	SO4	A	1549	-	4,4,4	0.17	0	6,6,6	0.12	0
4	SO4	A	1550	-	4,4,4	0.08	0	6,6,6	0.42	0
4	SO4	A	1551	-	4,4,4	0.18	0	6,6,6	0.23	0
4	SO4	A	1552	-	4,4,4	0.10	0	6,6,6	0.23	0
4	SO4	A	1553	-	4,4,4	0.21	0	6,6,6	0.47	0
4	SO4	A	1554	-	4,4,4	0.23	0	6,6,6	0.24	0
4	SO4	A	1555	-	4,4,4	0.15	0	6,6,6	0.36	0
4	SO4	A	1556	-	4,4,4	0.27	0	6,6,6	0.56	0
4	SO4	A	1557	-	4,4,4	0.11	0	6,6,6	0.10	0
2	LG9	B	1547	3	15,15,16	0.95	1 (6%)	17,22,24	2.54	6 (35%)
3	GLC	B	1548	2	12,12,12	0.66	0	17,17,17	1.06	1 (5%)
4	SO4	B	1549	-	4,4,4	0.13	0	6,6,6	0.33	0
4	SO4	B	1550	-	4,4,4	0.13	0	6,6,6	0.47	0
4	SO4	B	1551	-	4,4,4	0.25	0	6,6,6	0.28	0
4	SO4	B	1552	-	4,4,4	0.28	0	6,6,6	0.40	0
4	SO4	B	1553	-	4,4,4	0.29	0	6,6,6	0.42	0
4	SO4	B	1554	-	4,4,4	0.12	0	6,6,6	0.24	0
4	SO4	B	1555	-	4,4,4	0.15	0	6,6,6	0.41	0
4	SO4	B	1556	-	4,4,4	0.23	0	6,6,6	0.25	0
2	LG9	C	1547	3	15,15,16	0.94	0	17,22,24	2.44	6 (35%)
3	GLC	C	1548	2	12,12,12	0.66	0	17,17,17	1.03	1 (5%)
4	SO4	C	1549	-	4,4,4	0.13	0	6,6,6	0.41	0
4	SO4	C	1550	-	4,4,4	0.09	0	6,6,6	0.31	0
4	SO4	C	1551	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	C	1552	-	4,4,4	0.47	0	6,6,6	0.76	0
4	SO4	C	1553	-	4,4,4	0.15	0	6,6,6	0.23	0
4	SO4	C	1554	-	4,4,4	0.19	0	6,6,6	0.44	0
4	SO4	C	1555	-	4,4,4	0.14	0	6,6,6	0.26	0
2	LG9	D	1547	3	15,15,16	1.14	1 (6%)	17,22,24	2.23	6 (35%)
3	GLC	D	1548	2	12,12,12	0.58	0	17,17,17	0.89	0
4	SO4	D	1549	-	4,4,4	0.19	0	6,6,6	0.41	0
4	SO4	D	1550	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	D	1551	-	4,4,4	0.23	0	6,6,6	0.23	0
4	SO4	D	1552	-	4,4,4	0.21	0	6,6,6	0.45	0
4	SO4	D	1553	-	4,4,4	0.23	0	6,6,6	0.12	0
4	SO4	D	1554	-	4,4,4	0.21	0	6,6,6	0.33	0
4	SO4	D	1555	-	4,4,4	0.24	0	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	1556	-	4,4,4	0.17	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LG9	A	1547	3	-	0/4/33/36	0/2/2/2
3	GLC	A	1548	2	-	0/2/22/22	0/1/1/1
4	SO4	A	1549	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1550	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1551	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1552	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1553	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1554	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1555	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1556	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1557	-	-	0/0/0/0	0/0/0/0
2	LG9	B	1547	3	-	0/4/33/36	0/2/2/2
3	GLC	B	1548	2	-	0/2/22/22	0/1/1/1
4	SO4	B	1549	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1550	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1551	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1552	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1553	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1554	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1555	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1556	-	-	0/0/0/0	0/0/0/0
2	LG9	C	1547	3	-	0/4/33/36	0/2/2/2
3	GLC	C	1548	2	-	0/2/22/22	0/1/1/1
4	SO4	C	1549	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1550	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1551	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1552	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1553	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1554	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1555	-	-	0/0/0/0	0/0/0/0
2	LG9	D	1547	3	-	0/4/33/36	0/2/2/2
3	GLC	D	1548	2	-	0/2/22/22	0/1/1/1
4	SO4	D	1549	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1550	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1551	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	D	1552	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1553	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1554	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1555	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1556	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1547	LG9	C3-N4	-2.49	1.44	1.48
2	D	1547	LG9	C3-N4	-2.02	1.45	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1547	LG9	C6-C7-N4	-6.10	95.26	104.58
2	A	1547	LG9	C6-C7-N4	-5.09	96.80	104.58
2	D	1547	LG9	C6-C7-N4	-4.58	97.58	104.58
2	B	1547	LG9	C6-C7-N4	-4.05	98.39	104.58
2	C	1547	LG9	C2-C1-C9	-3.59	100.42	112.69
2	B	1547	LG9	C2-C1-C9	-3.18	101.84	112.69
2	A	1547	LG9	C2-C1-C9	-2.77	103.23	112.69
3	C	1548	GLC	C4-C3-C2	-2.53	106.37	110.84
2	C	1547	LG9	C1-C5-C4	-2.48	111.32	119.42
2	D	1547	LG9	C2-C1-C9	-2.09	105.57	112.69
2	D	1547	LG9	C1-C5-C4	-2.01	112.87	119.42
2	A	1547	LG9	C2-C1-C5	2.02	106.45	103.91
3	B	1548	GLC	O5-C5-C6	2.07	111.37	106.41
2	B	1547	LG9	C2-C1-C5	2.50	107.06	103.91
2	A	1547	LG9	C8-C7-C6	3.01	118.53	113.42
2	D	1547	LG9	C8-C7-C6	3.14	118.75	113.42
2	C	1547	LG9	C8-C7-C6	3.16	118.78	113.42
2	B	1547	LG9	C3-N4-C7	3.28	121.12	114.98
2	A	1547	LG9	C6-C4-C5	3.34	107.01	102.90
2	C	1547	LG9	C3-N4-C5	3.77	112.73	106.10
2	A	1547	LG9	C3-N4-C5	3.99	113.11	106.10
2	C	1547	LG9	C3-N4-C7	4.00	122.48	114.98
2	D	1547	LG9	C3-N4-C7	4.01	122.50	114.98
2	B	1547	LG9	C8-C7-C6	4.47	121.02	113.42
2	D	1547	LG9	C3-N4-C5	4.57	114.13	106.10
2	A	1547	LG9	C3-N4-C7	4.64	123.67	114.98
2	B	1547	LG9	C3-N4-C5	6.00	116.63	106.10



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1547	LG9	2	0
3	A	1548	GLC	1	0
4	A	1550	SO4	1	0
2	B	1547	LG9	2	0
4	B	1549	SO4	3	0
4	B	1550	SO4	1	0
4	B	1551	SO4	1	0
2	C	1547	LG9	1	0
4	C	1549	SO4	1	0
4	D	1549	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	506/535 (94%)	-0.48	5 (0%) 82 85	10, 18, 29, 50	0
1	B	503/535 (94%)	-0.58	9 (1%) 69 73	9, 16, 27, 40	0
1	C	501/535 (93%)	-0.43	13 (2%) 56 62	10, 18, 32, 43	0
1	D	503/535 (94%)	-0.39	12 (2%) 59 64	11, 20, 32, 46	0
All	All	2013/2140 (94%)	-0.47	39 (1%) 67 71	9, 18, 31, 50	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	SER	5.8
1	D	502	THR	5.4
1	C	513	PRO	4.9
1	D	292	PRO	4.4
1	C	104	GLY	4.4
1	C	502	THR	4.2
1	C	103	GLU	4.2
1	B	34	PRO	3.9
1	D	503	THR	3.9
1	A	132	ASN	3.8
1	C	512	TYR	3.7
1	B	544	ALA	3.7
1	D	544	ALA	3.5
1	C	84	ASN	3.3
1	C	545	THR	3.2
1	A	108	VAL	3.1
1	B	33	THR	3.1
1	B	545	THR	3.1
1	B	102	LYS	3.0
1	C	293	ASN	3.0
1	B	85	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	107	TYR	2.8
1	B	502	THR	2.8
1	A	36	THR	2.7
1	D	545	THR	2.6
1	C	503	THR	2.6
1	D	382	ASP	2.6
1	D	34	PRO	2.6
1	D	87	GLY	2.5
1	B	503	THR	2.5
1	C	536	GLU	2.4
1	D	293	ASN	2.3
1	B	513	PRO	2.3
1	A	507	GLY	2.2
1	C	382	ASP	2.2
1	D	513	PRO	2.2
1	C	105	GLU	2.2
1	C	383	GLN	2.0
1	D	537	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	1553	5/5	0.96	0.22	5.34	54,54,56,58	0
4	SO4	A	1555	5/5	0.93	0.20	4.05	56,58,58,59	0
4	SO4	C	1555	5/5	0.96	0.21	3.29	58,58,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	1556	5/5	0.97	0.21	2.00	44,44,46,47	0
4	SO4	A	1554	5/5	0.97	0.15	1.85	50,50,51,52	0
4	SO4	A	1556	5/5	0.87	0.21	1.71	53,54,55,55	0
4	SO4	C	1554	5/5	0.95	0.21	1.46	45,45,48,49	0
4	SO4	B	1556	5/5	0.96	0.22	1.39	42,43,45,46	0
4	SO4	B	1549	5/5	0.94	0.16	1.35	50,50,52,53	0
4	SO4	D	1550	5/5	0.99	0.16	1.24	53,54,54,55	0
2	LG9	A	1547	14/15	0.97	0.10	1.08	10,11,13,14	0
4	SO4	B	1551	5/5	0.97	0.18	0.69	42,44,44,45	0
4	SO4	D	1554	5/5	0.95	0.13	0.60	43,45,47,47	0
4	SO4	C	1552	5/5	0.95	0.11	0.60	25,26,30,33	0
4	SO4	D	1552	5/5	0.97	0.13	0.55	39,40,42,42	0
3	GLC	B	1548	12/12	0.98	0.09	0.43	9,11,12,14	0
2	LG9	B	1547	14/15	0.97	0.09	0.38	9,12,15,16	0
4	SO4	B	1555	5/5	0.94	0.14	0.15	48,48,50,51	0
2	LG9	C	1547	14/15	0.96	0.09	-0.06	9,12,14,18	0
3	GLC	A	1548	12/12	0.99	0.08	-0.40	10,12,13,15	0
3	GLC	C	1548	12/12	0.98	0.06	-0.59	10,11,15,17	0
4	SO4	A	1550	5/5	0.98	0.08	-0.61	27,28,34,34	0
4	SO4	B	1550	5/5	0.98	0.08	-0.62	32,32,34,35	0
4	SO4	B	1552	5/5	0.97	0.07	-0.67	28,30,30,31	0
4	SO4	A	1552	5/5	0.99	0.06	-0.79	28,28,31,31	0
3	GLC	D	1548	12/12	0.98	0.06	-0.82	10,13,14,14	0
4	SO4	C	1551	5/5	0.99	0.05	-0.88	33,34,35,35	0
2	LG9	D	1547	14/15	0.97	0.07	-0.91	10,12,14,16	0
4	SO4	A	1549	5/5	0.93	0.12	-1.07	78,78,79,79	0
4	SO4	C	1550	5/5	0.98	0.07	-1.15	33,35,37,39	0
4	SO4	C	1549	5/5	0.99	0.05	-1.19	26,26,30,30	0
4	SO4	A	1551	5/5	0.98	0.06	-1.39	28,29,31,31	0
4	SO4	D	1549	5/5	0.99	0.05	-1.44	28,30,30,30	0
4	SO4	D	1553	5/5	0.99	0.05	-1.59	26,30,33,33	0
5	CA	A	1558	1/1	0.96	0.04	-2.85	48,48,48,48	0
4	SO4	A	1553	5/5	1.00	0.04	-3.45	17,17,19,19	0
4	SO4	D	1551	5/5	0.93	0.21	-	55,55,57,57	0
4	SO4	D	1555	5/5	0.91	0.19	-	49,50,53,53	0
4	SO4	B	1554	5/5	0.92	0.25	-	71,72,72,73	0
4	SO4	A	1557	5/5	0.96	0.31	-	66,66,67,67	0
4	SO4	B	1553	5/5	0.93	0.13	-	41,43,46,46	0

## 6.5 Other polymers

There are no such residues in this entry.